

Numerical studies of Casimir interactions

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We study numerically the Casimir interaction between dielectrics in both two and three dimensions. We demonstrate how sparse matrix factorizations enable one to study torsional interactions in three dimensions. In two dimensions we study the full cross-over between non-retarded and retarded interactions as a function of separation. We use constrained factorizations in order to measure the interaction of a particle with a rough dielectric surface and compare with a scaling argument.

Dispersion forces have as their origin the fluctuations of polarization in materials coupled to the long-ranged electrodynamic interaction described by Maxwell's equations. The first convincing demonstration of their importance was the calculation by Keesom of the interaction between fluctuating classical dipoles [1]. The introduction of quantum fluctuations by London [2] accounted for the long-ranged, $1/r^6$, part of the van der Waals interaction in most materials. Later, Casimir and Polder [3] showed that retardation modifies the interactions in an important manner—leading to a decay in the interaction which is asymptotically $1/r^7$ at zero temperature. Further advances were made by the Russian school [4] who showed how to formulate the interactions in terms of the dielectric response of materials. Overviews with many references to theoretical and experimental developments are to be found in [5, 6, 7]. Retarded Casimir interactions are the dominant interaction between neutral surfaces at the submicron scale.

Whilst the analytic basis of the theory is largely established its application is difficult in experimentally interesting geometries. One is constrained to work with perturbative expansion about exactly solvable geometries [8], or use *ad hoc* schemes such as the proximity force approximation. Only a few geometries have been attacked with exact analytic techniques [9]. Recently several attempts have been made to study numerically the interactions by using methods from modern computational science— including fast multigrid lattice solvers [10] in order to calculate Green functions and forces, or the use of discretized determinants to determine free energies [11].

In this Letter we will present a series of techniques which enable one to evaluate the interaction between dielectric bodies in full vectorial electrodynamics. Firstly, we calculate the torsional potential between two three-dimensional bodies in the retarded regime, using a full discretization of Maxwell's equations, we note that the Casimir torque has recently received the attention of experimentalists [12, 13]. For more detailed studies we present results for two-dimensional systems. This allows us to study the cross-over between the near- and far-field regimes and also to measure the interaction between a particle and a rough surface. With these two-dimensional systems we implement general strategies which substantially increase the efficiency of simulations, at the same time decreasing the sensitivity of the results to numerical round-off errors.

In three dimensions we discretize Maxwell's equations to a cubic Yee-lattice [14], lattice constant $a = 1$, associating the electric degrees of freedom to the links, magnetic degrees of freedom are localized on the faces of the lattice. We remind the reader that the finite difference approximation to the $\nabla \times$ operator, here designated Curl , maps the electric field on four links surrounding the face of the cube to the magnetic field. Curl is needed in the Maxwell equation

$$\frac{\partial \mathbf{H}}{\partial t} = -c \text{Curl} \mathbf{E}$$

The adjoint operator maps fields from the faces to the links. We will denote it Curl^* . It intervenes in the second time dependent Maxwell equation.

$$\frac{\partial \mathbf{D}}{\partial t} = c \text{Curl}^* \mathbf{H}$$

The importance of clearly distinguishing the two operators will become apparent when we discuss the two-dimensional case below. We use Heaviside-Lorentz units in which Maxwell's equations are directly parameterized by the speed of light in vacuum, c .

From these two equations Lifshitz theory [15] shows that the free energy of interaction between dielectric bodies is found from the imaginary time wave equation for the vector potential in the temporal gauge where $\mathbf{E} = -\dot{\mathbf{A}}/c$ and $\phi = 0$

$$\left\{ \frac{\epsilon(\mathbf{r}, \omega) \omega^2}{\hbar^2 c^2} + \text{Curl}^* \text{Curl} \right\} \mathbf{A} = \mathcal{D}_A \mathbf{A} = 0$$

Alternatively one introduces a magnetic formulation and works with a potential such that $\mathbf{H} = \dot{\mathbf{G}}/c$ and considers the wave equation

$$\left\{ \frac{\omega^2}{\hbar^2 c^2} + \text{Curl} \frac{1}{\epsilon(\mathbf{r}, \omega)} \text{Curl}^* \right\} \mathbf{G} = \mathcal{D}_G \mathbf{G} = 0$$

In our work we always consider the differences in free energy between pairs of configurations; we thus avoid a full account of the self-energy variations of dielectric media [11]. The free energy difference between two configurations 1, 2 is found from

$$U^{1,2} = \int_0^\infty \frac{d\omega}{2\pi} \{ \ln \det \mathcal{D}^1(\omega) - \ln \det \mathcal{D}^2(\omega) \} \quad (1)$$

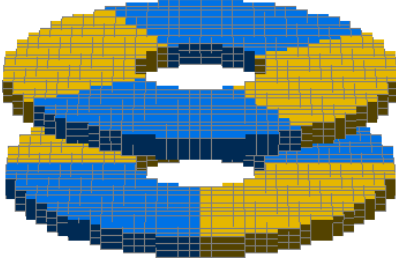


FIG. 1: A Pair of structured dielectric rings. Each quadrant has different dielectric properties.

for either choice of wave operator, \mathcal{D}_A or \mathcal{D}_G ; while self-energy contributions are different in the two formulations we have verified with our codes that both give the same result for the long-ranged part of the interactions that we are interested in.

We perform the frequency integration in eq. (1) by changing integration variables to z , where $\omega = \alpha z / (1 - z)$ with $0 < z < 1$. The parameter α is chosen so that the major features in the integrand occur for values of z near $1/2$. We then use N_g -point Legendre-Gauss quadrature to replace the integral by a weighted sum over discrete frequencies. We evaluate determinants by finding the Cholesky factorization L_D of $\mathcal{D}(\omega)$ such that L_D is lower triangular [16] and $L_D L_D^T = \mathcal{D}(\omega)$. The determinant of \mathcal{D} is then given by

$$\ln \det \mathcal{D}(\omega) = 2 \sum_i \ln (L_{D,i,i})$$

When we examine the detailed structure of Maxwell's equations discretized to $V = L^3$ sites in three dimensions we discover that the Curl operator is a matrix of dimension $3V \times 3V$ and has $12V$ non-zero elements. The operator (Curl* Curl) has $39V$ non-zero elements. The major technical difficulty comes from the fact that the matrices we work with have dimensions which are very large, $\sim 10^6 \times 10^6$. All numerical work was performed with an Intel Xeon-5140 workstation.

We now calculate the Casimir torque between two parallel rings centered on a common axis, figure 1. Each ring is divided into quadrants with alternating dielectric properties. We take permittivities which are independent of frequency, corresponding to the full retarded regime [15] with $\epsilon_1(\omega) = 5$, $\epsilon_2(\omega) = 10$; the space around the rings is a vacuum with $\epsilon_r = 1$. We measure the energy of interaction as the top ring is rotated with respect to the lower. The zero of the interaction corresponds to aligned rings. As the rings are rotated the interface between the dielectric materials, as interpolated to the lattice, undergoes some re-arrangement changing the self energy of the rings. We thus perform two runs. The first run of a single rotating ring determines this variation in the self-energy. The second run with the both rings allows one to measure the interaction energy by subtraction.

We worked with a system of dimensions $V = 55 \times 55 \times 55$, figure 2. The graph of the interaction energy as a function of

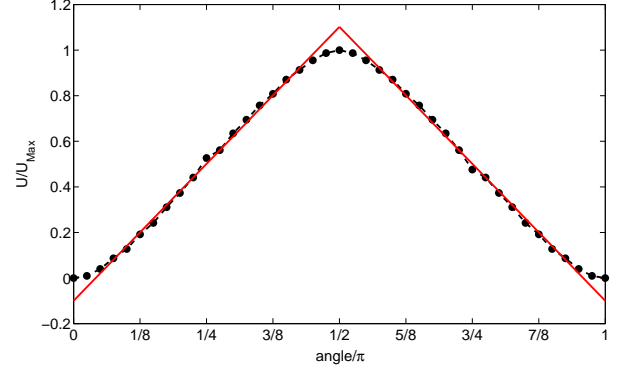


FIG. 2: Interaction energy as a function of angle as a ring of figure 1 rotates. In the linear parts of the curve the torque is almost independent of the angle. Ring diameter $36a$, separation and thickness $2a$. Rounding is determined by the ratio of separation to diameter of the rings. 10 days of computation with $N_g = 8$. Cholesky factor 9GB.

angle is noticeably triangular in shape between $\pi/8$ to $3\pi/8$. This is understood by the fact that the interaction energy is dominated by the interactions directly across the gap. The fluctuations in the curve about the expected linear behavior, together with its slight asymmetry give an idea of the noise coming from irregularities of the interpolation of the disks to the lattice. This irregularity is particularly clear on comparing the points for $\pi/4$ and $3\pi/4$.

We now turn to two-dimensional electrodynamics where we can study systems with larger linear dimensions. Such large system sizes are needed in order to follow the cross-overs between different regimes in the interaction of particles or if one wishes to simulate structured or disordered materials in order to understand the efficiency of analytic approximations.

In three dimensions the two formulation in terms of \mathcal{D}_A and \mathcal{D}_G are largely equivalent. In two-dimensional electrodynamics this is no longer the case. Consider an electrodynamic system in which there are two components of the electric field in the $x - y$ plane; the magnetic field then has just a single component in the z direction. The Curl operator becomes a *rectangular matrix* of dimensions $V \times 2V$ where now $V = L^2$. The standard formulation in terms of the vector potential gives to an operator \mathcal{D}_A of dimensions $2V \times 2V$ with $14V$ non-zero elements; the alternative formulation in terms of \mathcal{D}_G leads to determinants of dimensions $V \times V$ involving just $5V$ non-zero elements; the size of the matrix that we must work with is smaller in the \mathcal{D}_G formulation. We used \mathcal{D}_G in the following numerical work, having checked that we obtain equivalent results.

We started by measuring the cross-over between the short-ranged non-retarded interaction to the long-ranged Casimir force. We studied a pair of dielectric particles described by

the single pole approximation to the dielectric constant

$$\epsilon(\omega) = 1 + \frac{\chi}{1 + \omega^2/\omega_0^2\hbar^2}$$

where χ is the zero frequency electric susceptibility. The interaction is retarded for separations $D \gg c/\omega_0$, non-retarded for $D \ll c/\omega_0$.

We measured the interaction between two dielectric particles in a square, periodic cell of dimensions $L \times L$ using SuiteSparse [17] to perform both the ordering and the factorization of the matrices. We placed a first particle at the origin, and considered two possible positions of a second particle to calculate a free energy difference using eq. (1). The first results were disappointing—rather small systems ($L = 50$) were sensitive to numerical round-off errors. The origin of this problem was quite clear. In a large system there is an extensive self-energy $\sim L^2$. Pair interactions calculated as the difference between two large numbers are unreliable.

We avoided this problem by separating the free energy contributions from the neighborhood of the three interesting sites and the rest of the system. We did this by introducing a block-wise factorization of \mathcal{D} that enabled us to both solve the round-off problem while re-using much of the numerical effort need to generate the Cholesky factors thus improving the efficiency of the code.

We now write the symmetric matrix from the wave equation in block form, $\mathcal{D} = \begin{pmatrix} X & Y \\ Y^T & Z \end{pmatrix}$. Its determinant is $\det(\mathcal{D}) = \det(X)\det(S)$ where the Schur complement $S = Z - Y^T X^{-1}Y$ [18]. We group sites so that the great majority is within the block X and sites that we are interested in are in the block Z . It is the term in $\det(X)$ that gives the large extensive free energy which caused our numerical problems. It is independent of the properties of our test particles. All the interesting information on energy differences is in the Schur complement, S .

We start by finding the Cholesky factorization of X , L_x . The Schur complement is calculated by solving the triangular equations $L_x U = Y$ by forward substitution, then calculating $S = Z - U^T U$. Our separation of energies into an extensive constant and a small set of interacting sites allows us to study the interaction of systems of sizes up to $L = 2000$ before round-off becomes a problem.

In order to generate data we generalized the method to a three level scheme—firstly collect the set of sites (here ~ 100) of all the separations required to generate a curve into the block Z , and form the Schur complement forming a small effective theory for all these remaining sites. Within the smaller matrix that has been generated we again re-order to successively put each interesting sets of variables in the bottom-right corner of the effective theory and find the Schur complement of these remaining variables. We can then calculate interactions between the particles while minimizing round-off errors.

We remind the reader that in two dimensions the electrostatic potential is logarithmic between two charges, and that dipole-dipole fluctuations lead to van der Waals interactions

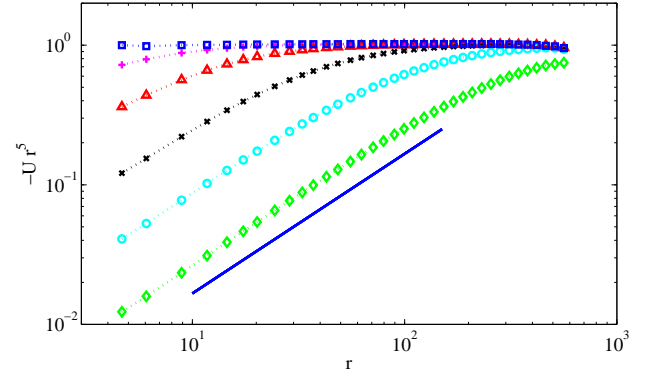


FIG. 3: Scaled interaction free energy, $-U r^5$ for a pair of dielectric particles ($\epsilon(0) = 8$) in a box of dimensions 2000×2000 as a function of separation. Curves from top to bottom correspond to $\omega_0/c = 10, 0.3, 0.1, 0.03, 0.01, 0.003$. For large ω_0/c , $U r^5$ is constant, \square . For smaller ω_0/c we see both retarded and non-retarded interactions. Solid line corresponds to $U_{vdw} \sim 1/r^4$. 10GB for Cholesky factor. Six hours of calculation. $N_g = 25$.

decaying as $U_{vdw} = 1/r^4$. As in three dimensions retardation leads to an accelerated decay so that the Casimir interaction varies as $U_c \sim 1/r^5$. In our simulations we used values of ω_0/c varying from 0.003 to 10, figure 3. We determined the energy of interaction of particles U , as a function of separation r while moving the second particle in the simulation cell out to $(L/5, L/5)$; the zero of energy is calculated for two particles separated by $(L/2, L/2)$. We scale out the retarded behavior, plotting $-U(r)r^5$. We see that for the largest ω_0/c the interactions are retarded for all separations, \square . For the smaller values of ω_0/c the interaction varies as $1/r^4$. In the scaled curve this gives the linear rise clearly visible in the figure, \diamond . For $0.1 < \omega_0/c < 0.01$ we see both the near- and far-field behaviors clearly displayed within a single sample—permitting the detailed study of cross-over phenomena with frequency dependent dielectric behavior. No assumptions of symmetry are made in the calculation; the method can be used with bodies of arbitrary geometry.

We now turn to a problem where analytic results are much more difficult to find: The interaction of a dielectric particle with a rough surface, figure 4. We generated rough surfaces as realizations of solid-on-solid random walks on a lattice. Approximately half of the simulation box contains dielectric material with $\epsilon = 8, \omega_0 = \infty$; the rest of the box has $\epsilon = 1$. We measure the interaction with a test particle as a function of the distance from the rough surface using the above method of block Schur complements to perform a single large factorization per frequency for each realization of the disorder. We generated 1000 rough surfaces and measured the average interaction with the surface $\langle U \rangle$, as a function of separation, as well as the variance in the potentials.

We understand the results, figure 5, with a scaling argument. When the particle is a distance r from the surface the interaction is dominated by a front of length r along the surface. Since the surface is a random walk its average posi-

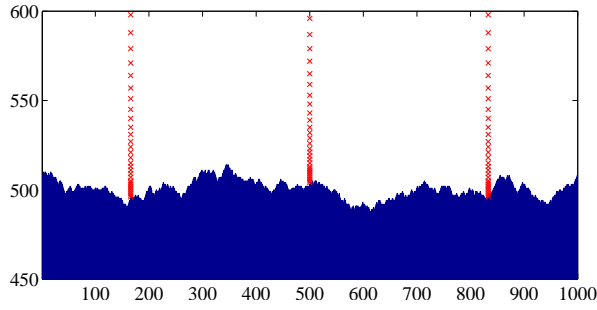


FIG. 4: Realization of rough interface and set of measurement positions, \times , for the interaction energy which will be separated into the block Z . Anisotropic horizontal and vertical scales.

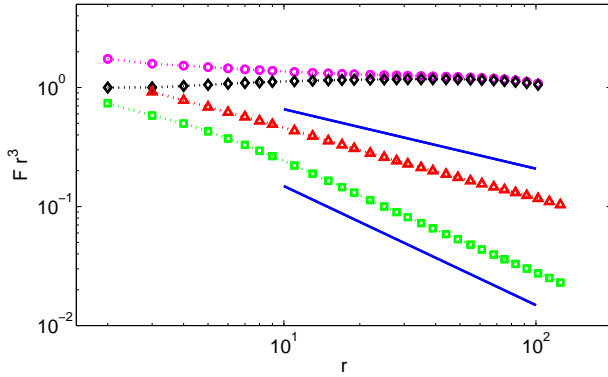


FIG. 5: (1) \circ , $-\langle U \rangle r^3$, averaged interaction between dielectric particle and rough dielectric surface. (2) \diamond , $-U_s r^3$, interaction between particle and flat surface. (3) \triangle , $\sigma_u r^3$, variance of interaction for rough surfaces. (4) \square , $\delta U r^3$, difference in mean interaction energy between a flat and a rough surface. Solid lines: $r^{-3.5}$ and r^{-4} . $L = 1000$. Two weeks of simulation time. Cholesky factor 2.5GB. $N_g = 20$.

tion is displaced by $\delta r \sim \pm r^{1/2}$ compared to the flat surface. The interaction between a smooth surface and a particle varies as $U_s \sim 1/r^3$ in the Casimir regime. The interaction of the particle should thus be $U \sim 1/(r + \delta r)^3$. If we expand to first order we find that the variance of the interaction should scale as, $(\triangle) \sigma_u \sim r^{-3.5}$ while the second order expansion gives a shift in the mean potential, $\langle U \rangle$, which varies as, $(\square) \delta U \sim 1/r^4$. The numerical data are compatible with this scaling. The argument is easily generalized to affine surfaces with other, less trivial roughness exponents giving results compati-

ble with [19].

We have demonstrated the power of direct methods from linear algebra when applied to the study of dispersion forces. In three dimensions we have measured interactions in experimentally realizable geometries—though system sizes are still too small to accurately measure cross-overs between different scaling regimes. In two dimensions we have shown how to measure the cross-over between London dispersion and Casimir interactions, and have determined correction to scaling exponents for the interactions of a disordered systems.

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